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DYNAMICS OF IMPURITY SPIN ABOVE THE KONDO TEMPERATURE I
CALCULATION OF THE SPIN PROPAGATOR AND THE STATIC SUSCEPTIBILITY

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BUDAPEST

DYNAMICS OF IMPURITY SPIN ABOVE THE KONDO TEMPERATURE I. CALCULATION OF THE SPIN PROPAGATOR AND THE STATIC SUSCEPTIBILITY.

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Summary++

The dynamics of impurity spin contained by nonmagnetic host metal is investigated theoretically. The pseudofermion representation proposed by Abrikosov is applied to impurity spin. The calculations are carried out keeping only the leading logarithmic terms in any order of the perturbation theory. This approximation is adequate only above the Kondo temperature. Abrikosov's method is slightly modified to treat the spin dynamics. The real and the imaginary part of the pseudofermion self-energy is calculated. The imaginary part of the self-energy satisfies a simple relation which holds between the electron and pseudofermion self-energies. The decrease in the effective gyromagnetic factor is determined, which shows how the spin compensated state begins to form at low temperature. The first terms of the power series of the static susceptibility calculated from the pseudofermion Green function are in agreement with the results of the previous perturbative calculations given by e.g. Yosida and Okiji. The spectral function of the pseudofermion propagator is discussed in details. It has a long tail at large positive energies and satisfies the sum rule $\int_{-\infty}^{\infty} d\omega \rho(\omega) = 1$. The dynamic susceptibility and other physical quantities will be presented in the second part of this paper.

1. Introduction

Recently the static and dynamic susceptibilities of dilute alloys have attracted great interest. In the case of magnetic impurities in nonmagnetic host metals the interaction between the impurity spins and the conduction electrons exhibits some anomalous behaviour, called Kondo [1] effect. These anomalies are connected with the formation of a spincompensated state built up by the impurity spin and the conduction electrons. The problem has frequently been attacked from the side of static and dynamic susceptibilities. The formation of the spincompensated state would mean a reduction in the static and some deviation in the dynamic susceptibilities.

In the mathematical formulation of the theory a characteristic temperature /Kondo temperature/ appears. Well above this temperature the perturbation theory leads to correct results, but this situation changes essentially as this temperature is approached and below. The present treatment is restricted to the temperature region well above the Kondo temperature.

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Calculations have been carried out by several authors to determine the static susceptibility up to the first few orders of the perturbation theory. Some of these works [2,3] are based on the Kondo Hamiltonian, while the others [4-7] on the Anderson model. These calculations yield similar results, for there is some relation between these two models. [8,9] Considering the low temperature region there are further approaches which start with some trial wave function. [10-14]

The result, derived by Hamann [15] on the basis of Nagaoka's decoupling scheme [16] worked out for the Green's function equations, covers the whole region of temperature. These results are in agreement with the perturbative treatment in the high temperature limit, but this agreement is restricted to the highest power of the logarithmic terms in any order of the perturbation theory.

Recently also the dynamic susceptibility [17-21] has been investigated. Unfortunately all these calculations are limited to not higher than the third order in the exchange coupling concerning the self-energy. Spencer and Doniach [17] pointed out first, having carried out the calculations up to the second order that a typical logarithmic term appears in the expression of the g-shift. Wang and Scalapino [18] have derived a similar g-shift and a HlogH term for the linewidth in the high external magnetic field limit.

The difficulties of calculating the dynamical susceptibility are due to the limited possibilities in the application of diagram techniques and linked cluster expansion for spin variables. Spencer and Doniach [17] have made use of a pseudofermion representation of the spin variables valid for S=1/2. Wang and Scalapino [18] have applied a diagram technique proposed by Wang and Callen [22-23] for arbitrary spin, but unfortunately this method works in a simple way only in the high magnetic field and low temperature limit.

The study of the dynamics of impurity spins is of particular interest. Until now, only the dynamics of electrons has been investigated in details. Abrikosov has neglected the renormalization of pseudofermions in his earlier works [24-25], for it does not contribute to the dynamics of electrons within logarithmic accuracy. Suhl [26] considered only the one electron intermediate states studying the Chew-Low equations.
In the dynamics of impurity spins those intermediate states play an important role, which contain at least two electrons and one hole.

The aim of the present paper is to investigate the dynamics of spins considering only the highest power of logarithmic terms in any order of

the perturbation theory. Abrikosov's pseudofermion representation of spin variables is applied. In the first paper we concentrate on the calculation of the pseudofermion propagator and the static susceptibility, while in the second paper the dynamic susceptibility is calculated.

In Sec. 2. Abrikosov's pseudofermion representation of spins and his diagram method [24] is slightly modified. This modification stands the critics [27] which has been directed against some difficulties connected with the applicability of the linked cluster theorem due to the occurence of some unphysical quantummechanical states in Abrikosov's representation.

Previously Abrikosov [24-25] has calculated the electron self-energy. In these calculations only those values of the vertex function have been used in which the energy variables of the pseudofermions were approximately zero. The general form of the vertex function for all regions of the energy variables is not available. In Sec. 3. a few remarks are made about the vertex function which give the possibility for carrying out the further calculation in the logarithmic approximation [28]. In the latter approximations only the highest power of the appearing logarithmic terms is treated in every order of the perturbation theory.

The real and the imaginary parts of the pseudofermion self-energy are calculated in Sec. 4. Determining the real part of the self-energy near the resonance energy two terms are obtained, one term is proportional to the external magnetic field while the other one to the energy. Both of these terms contain a typical logarithmic expression characteristic for the Kondo effect, which diverges at the Kondo temperature. Due to the appearance of this divergency the validity of our treatment is restricted to the temperature region well above the Kondo temperature. The term proportional to the magnetic field results in a shift of the gyromagnetic factor of the impurity spin, which shift describes the compensation of the moment of the impurity by the magnetically polarized electron cloud around the impurity. This compensation becomes more and more effective as the Kondo temperature is approached. This result which is valid only above the Kondo temperature, gives a hint that at zero temperature the impurity moment might be totally screened by the surrounding polarized electron cloud and a so called compensated bound state of the impurity and one or more conduction electrons and holes might be formed. The second term of the real part of the self-energy which is proportional to the energy leads to a renormalization factor in the pseudofermion Green's function. The appearance of this renormalization factor will be very important in the study of the impurity spectral function. Furthermore the renormalization constant can be included into a temperature dependent effective exchange

coupling constant which may be of fundamental importance in the Kondo problem.[29]

The relaxation rate of the conduction electrons scattered by the paramagnetic impurities was the first physical quantity in which the Kondo anomaly has been found. Approaching the Kondo temperature by lowering the temperature, the relaxation rate increases. It is reasonable to expect that a similar behaviour is shown by the relaxation rate of the impurity spin, as it is really found is Sec. 4. It is pointed out that the pseudofermion and electron relaxation time satisfy an identity which is derived by counting the number of collisions in two different ways.

The spectral function of the pseudofermion propagator is derived in Sec. 5. It turns out that besides a Lorentzian contribution to the spectral function another term becomes important especially at large positive energy values. This second term exhibits a long tail character. The calculated spectral function satisfies the sum rule $\int_{-\infty}^{\infty} d\omega \rho(\omega) = 1$ and this seems to be a good check for the calculated self-energy which determines the spectral function. It will be shown in the second part of this paper that the long tail part of the spectral function is of particular interest in studying the dynamical susceptibility.

The static susceptibility is obtained from the one particle pseudofermion Green's function in Sec.7. The first few terms in the power expansion of the static susceptibility with respect to the exchange coupling reproduce the results obtained earlier by applying perturbation method [2-6]. As far as we know, this calculation is the first one which gives the leading logarithmic terms of the static susceptibility up to arbitrary orders in the exchange coupling constant. This result corresponds to a modified Curie law with a renormalized, temperature dependent effective gyromagnetic factor.

In the second part of this paper the dynamic susceptibility will be calculated. The possible importance of the spin dynamics in the treatment of the Kondo problem, which has not yet been sufficiently considered in details, is the subject of another paper [29].

2. Abrikosov's pseudofermion representation of impurity spin and its modification

Abrikosov [24] has applied a pseudofermion representation of spin operators to the treatment of the Kondo effect. This calculation has been carried out to logarithmic accuracy. Calculating the electron self-energy

in this approximation the self-energy of the pseudofermions can be neglected In this work we calculate the pseudofermion propagator to construct the spin correlation functions. The unphysical states containing more or less than one pseudofermion particles per impurity are separated by introducing the pseudofermion energy, λ which tends to infinity. The many pseudofermion states are cancelled by this procedure. The remaining states have been normalized by the normalization factor $e^{\lambda/T}.\ (2S+1)^{-1}$ in Abrikosov's works. This normalization factor has to be modified due to the pseudofermion self-energy, which has been neglected before. The correct normalization procedure is presented in this section keeping our eye on the applicability of the linked cluster theorem. An electron gas and one localized spin is considered. The system is described by the Hamiltonian

$$H = H_o + H_{int} \qquad /1/$$

where

$$H_o = \sum_{p,\alpha} \varepsilon(\bar{p})\ a^+_{\bar{p},\alpha}\ a_{\bar{p},\alpha} - \mu_B\ H \sum_{\bar{p},\alpha,\alpha'} a^+_{\bar{p},\alpha}\ \sigma^z_{\alpha\alpha'}\ a_{\bar{p},\alpha'} + g\mu_B\ H\ S^z \qquad /2/$$

and

$$H_{int} = -\frac{J}{N} \sum_{\alpha\beta} \psi^+_\alpha\ (\bar{R})\ \sigma_{\alpha\beta}\ \psi_\beta\ (\bar{R})\ \bar{S} \qquad /3/$$

In these formulas ψ^+ and ψ are the electron field operators taken at the impurity site, $\bar{R}$, $a^+_{p,\alpha}$ and $a_{p,\alpha}$ are the creation and annihilation operators corresponding to momentum p, and spin α, $\bar{\sigma}$ and $\bar{S}$ are the Pauli matrix and the impurity spin operator, resp., $\frac{J}{N}$ denotes the coupling constant of the s-d interaction, $\varepsilon(\bar{p}) = p^2/2m - \mu$ is the free electron energy, H is the magnetic field with direction -z, μ_B is the Bohr magneton, and g is the gyromagnetic factor of the impurity spin. It is supposed that the gyromagnetic factor of the electrons is $g_e = 2$.

Abrikosov has introduced the following representation for the impurity spin operators

$$\bar{S} = a^+_\beta\ \bar{S}_{\beta\beta'}\ a_{\beta'} \qquad /4/$$

where a_β^+ and a_β are the pseudofermion operators, and $S_{\beta\beta'}$ is the spin matrix.

Using Abrikosov's technique fictitious states occur, which contain more or less than one pseudofermions. The fictitious states containing more than one pseudofermions can be eliminated by introducing a pseudofermion „kinetic energy", λ which tends to infinity. On the other hand let us suppose that the states which do not contain any pseudofermions do not occur in the calculations. This will be proved to be true in the actual calculations of the present paper. It is due to the fact that special problems are investigated, namely the spin correlation functions. Some short remarks will be done for the general case at the end of the present section.

The density operator to be applied is

$$\rho = \exp\{-\beta H'\}$$

where the Hamiltonian H' contains the "kinetic energy" of the pseudofermions, too: i.e. $H'=H+H_\lambda$ and $H_\lambda = \lambda \sum_\beta a_\beta^+ a_\beta$.

Considering the physical states only, the probability that one pseudofermion state is occupied, is as follows

$$\langle N_s \rangle^{phys} = \langle \sum_\beta a_\beta^+ a_\beta \rangle^{phys} = Tr^{phys}(N_s \rho) \qquad /5/$$

where the operation Tr^{phys} means, that the trace is restricted to the physical states. Neglecting the exchange Hamiltonian (3) this probability is $(2S+1)\, e^{-\lambda/T}$.

The expectation value of a physical quantity A taken over the physical states, can be written as

$$\langle A \rangle^{phys} = \frac{Tr^{phys}(\rho A)}{Tr^{phys}(\rho)} \qquad /6/$$

The factors $e^{-\lambda/T}$ occuring in the nominator and denominator of (6) cancel each other, hence (6) is independent of λ .

Making use of the assumption that the states, with no pseudofermion do not give contribution to the matrix elements of the operator ρA, the trace in formula (6) can be extended to all states /physical and fictitious/

$$\langle A \rangle^{phys} = \lim_{\lambda \to \infty} \frac{Tr(\rho A)}{Tr\,(\rho N_s)} \qquad /7/$$

In order to eliminate from the denominator the states which do not contain any pseudofermions, the limit $\lambda \to \infty$ is taken and the normalization factor is completed by the pseudofermion number operator, N_s.

The expression (7) can be written in another form, too,

$$\langle A \rangle^{phys} = \lim_{\lambda \to \infty} \frac{\frac{Tr(\rho A)}{Tr(\rho)}}{\frac{Tr\,(\rho N_s)}{Tr(\rho)}} = \lim_{\lambda \to \infty} \frac{\langle A \rangle_\lambda}{\langle N_s \rangle_\lambda} \qquad /8/$$

where the notation

$$\langle x \rangle_\lambda = \frac{Tr\,(\rho x)}{Tr\,(\rho)} \qquad /9/$$

has been used. The latter expectation value can be calculated using the linked cluster theorem, because there is no restriction to the physical states. Therefore the nominator and denominator of the formula [8] have to be calculated separately and the linked cluster theorem can be applied to the calculations of both quantitites.
This procedure will be applied in the present paper.

In the general case the states which do not contain any pseudofermions might contribute to the expectation value $\langle A_\lambda \rangle$ in its nominator, $Tr(\rho A)$ This difficulty can be avoided, if the operator A is replaced by AN_s and then we have the following exact formula

$$\langle A \rangle^{phys} = \lim_{\lambda \to \infty} \frac{\langle AN_s \rangle_\lambda}{\langle N_s \rangle_\lambda} \qquad /10/$$

The actual calculation of this formula seems to be not easy. It is worth mentioning that there are other possibilities, too, see Appendix I.

3. On the off energy shell vertex function

Abrikosov [24] has calculated the electron lifetime up to the logarithmic accuracy. In his calculations the electron-pseudofermion vertex function has been needed only when the energies of the pseudofermions were on the energy-shell. In the present investigation of the dynamics of localized spins the off-energy shell vertex function plays an important role, and this vertex is not available for the whole range of its arguments even in logarithmic approximation. In this section the off-energy shell vertex function is calculated with logarithmic accuracy closely following Abrikosov's original treatment, but only in some restricted range of the arguments.

The diagram corresponding to the vertex function $\Gamma_{\alpha\beta\alpha'\beta'} \cdot (i\varepsilon, i\omega_1 | i(\varepsilon+\omega_1-\omega_2), i\omega_2)$ can be seen in Fig. 1/a. where the solid and dotted lines stand for the electrons and pseudofermions, resp. and $\omega = \pi T(2n+1)$. The vertex function may be written as a sum given in Fig. 1/b in the graphical form, where Λ_1 and Λ_2 can be cut into two parts by cutting one electron and one pseudofermion line which are parallel or antiparallel, resp. This type of separation of the vertex function

$$\Gamma = \frac{J}{N} + \Lambda_1 + \Lambda_2 \qquad /11/$$

is correct only in the logarithmic approximation.

The vertex parts Λ_1 and Λ_2 can be regarded as functions of a single energy variable, which are the sum or the difference of the incoming electron and pseudofermion energy variables, if all the energy variables are smaller than the considered one variable or at least they are of the same order of the magnitude. Abrikosov has derived equations for these vertex parts and these equations are graphically represented in Fig. 2/a-b and their algebraic forms are as follows

$$\Lambda_{1\alpha\beta\alpha'\beta'}(\omega) = \rho_o \int_{|\omega|}^{D} \frac{d\tilde{\omega}}{\tilde{\omega}} \Gamma_{\alpha\beta\alpha''\beta''}(\tilde{\omega}) \Gamma_{\alpha''\beta''\alpha'\beta'}(\tilde{\omega}) \qquad /12/$$

and

$$\Lambda_{2\alpha\beta\alpha'\beta'}(\omega) = -\rho_o \int_{|\omega|}^{D} \frac{d\tilde{\omega}}{\tilde{\omega}} \Gamma_{\alpha\beta\alpha''\beta''}(\tilde{\omega}) \Gamma_{\alpha''\beta''\alpha'\beta'}(\tilde{\omega}) \qquad /13/$$

where

$$\Gamma_{\alpha\beta\alpha'\beta'}(\tilde{\omega}) = (\bar{\sigma}_{\alpha\alpha'}, \bar{s}_{\beta\beta'}) \frac{\frac{J}{N}}{1 + 2\frac{J}{N}\rho_o \log \frac{D}{|\tilde{\omega}|}} \qquad /14/$$

Here $\rho_o = \frac{p_o m}{2\pi^2}$ is the density of states at the Fermi energy for a definite spin direction, m is the electron mass, p_o is the Fermi momentum and D is the cut-off energy.
Making use of the identities

$$(\bar{\sigma}_{\alpha\alpha''} \bar{s}_{\beta\beta''})(\bar{\sigma}_{\alpha''\alpha'} \bar{s}_{\beta''\beta'}) = s(s+1)\, \delta_{\alpha\alpha'} \delta_{\beta\beta'} - (\bar{\sigma}_{\alpha\alpha'} \bar{s}_{\beta\beta'}) \qquad /15/$$

and

$$(\bar{\sigma}_{\alpha\alpha''} \bar{s}_{\beta''\beta'})(\bar{\sigma}_{\alpha''\alpha'} \bar{s}_{\beta\beta''}) = s(s+1)\, \delta_{\alpha\alpha'} \delta_{\beta\beta'} + (\bar{\sigma}_{\alpha\alpha'} \bar{s}_{\beta\beta'}) \qquad /16/$$

and carrying out the integrations in eq. /II/ and /12/ the following results are obtained

$$\Lambda_{1\alpha\beta\alpha'\beta'}(\omega) = -\frac{J}{2N}\left[s(s+1)\, \delta_{\alpha\alpha'} \delta_{\beta\beta'} - (\bar{\sigma}_{\alpha\alpha'} \bar{s}_{\beta\beta'})\right] \cdot$$

$$\cdot \left\{ \frac{1}{1 + 2\frac{J}{N}\rho_o \log \frac{D}{|\omega|}} - 1 \right\} \qquad /17/$$

and

$$\Lambda_{2\alpha\beta\alpha'\beta'}(\omega) = \frac{J}{2N}\left[s(s+1)\, \delta_{\alpha\alpha'} \delta_{\beta\beta'} + (\bar{\sigma}_{\alpha\alpha'} \bar{s}_{\beta\beta'})\right] \cdot \qquad /18/$$

$$\cdot \left\{ \frac{1}{1 + 2 \frac{J}{N} \rho_o \log \frac{D}{|\omega|}} - 1 \right\} \qquad /18/$$

If the argument in this expressions is smaller than the thermal energy, kT, then this argument has to be replaced by kT on the left hand sides of eqs. /17/ and /18/.

The crucial point of this approximations is the choice of the arguments for the two vertices appearing in eqs. /12/ and /13/ (or in Fig.s. 2/a-b). The calculation of the closed loop between the vertices results in a limitation of the variables in the other logarithmic integrals occuring in the vertices, and these limitations have been considered in eqs. /12/ and /13/. In the calculation e.g. of the vertex on the left hand side in Fig. 2/a, if $|\varepsilon - \omega_1| >> |\varepsilon + \omega_1|$ another restriction may arise, too. In this case there is a relatively large energy transfer through the vertex compared to the transfer through the cut. This large energy transfer causes a higher value of the lower limit in the logarithmic integrals of this vertex and for this reason the expression $\log \frac{D}{|\tilde{\omega}|}$ in $\Gamma(\tilde{\omega})(\tilde{\omega} = |\varepsilon + \omega_1|)$ has to be replaced by $\log \frac{D}{|\varepsilon - \omega_1|}$ for $|\varepsilon - \omega_1| > |\varepsilon + \omega_1|$.

Therefore Abrikosov's results /eqs. /11-14/ are correct only if there is not a larger[x] energy transfer through some of the vertices in Fig. 2/a-b than the transfer at the cut.

4. Pseudofermion self-energy

The free pseudofermion and electron propagators are

$$\mathcal{G}^{(o)}_{\alpha\alpha'}(i\omega_n) = \frac{1}{i\omega_n + g\mu_B H M_\alpha - \lambda} \delta_{\alpha\alpha'} \qquad /19/$$

and

$$\mathcal{G}^{(o)}_{\alpha\alpha'}(p, i\omega_n) = \frac{1}{i\omega_n - \xi_{\bar{p}} + \mu_B H \sigma^z_{\alpha\alpha'}} \delta_{\alpha\alpha'} \qquad /20/$$

where $\xi_{\bar{p}} \simeq \frac{p^2}{2m} - \mu$ is the kinetic energy, μ is the chemical potential and M_α is the z component of the localized spin. The magnetic

Footnote: [x] This comparison is made on the basis of the order of magnitudes.

field H is directed to the negativ z direction. In the calculation of the pseudofermion self-energy to logarithmic accuracy the electron self-energy correction may be neglected. This can be seen in a similar way as in the case, where the pseudofermion renormalization does not contribute to the electron selfenergy in the logarithmic approximation as it has been pointed out by Abrikosov [24]. The electron energy shift $\mu_B H\sigma^z$ caused by the external magnetic field may be transformed out for all of the internal electron lines in the framework of the logarithmic approximation / see ref. [25]/.

The renormalized pseudofermion propagator can be written as

$$\mathcal{G}_{\alpha\alpha'}(i\omega_n) = \frac{\delta_{\alpha\alpha'}}{i\omega_n + g\mu_B M_\alpha H - \lambda - \Sigma_\alpha(i\omega_n) + 2\frac{J}{N}\rho_o \mu_B M_\alpha H} \qquad /21/$$

where $\Sigma_\alpha(i\omega_n)$ denotes the self-energy disregarding the correction corresponding to the simple electron bubble illustrated in Fig.3. which correction has to be added to the self-energy. This separation is reasonable, because the latter describes the paramagnetic Knight shift.

The real and imaginary part of the self-energy will be calculated successively since different approximations have to be applied.

a. Real part of the self-energy

The present calculations have been carried out for small external magnetic field, $g\mu_B H << kT$.

The general self- energy diagram is given in Fig.4. Its contribution cannot be calculated in a straightforward way, because the value of the vertex function in the presence of an external magnetic field is not available. To work out an appropriate approximation we calculate first the second order diagram. This diagram can be seen in Fig.5. and its contribution is as follows

$$\Sigma^{(2)}_{\alpha\alpha'}(i\omega) = -\left(\frac{J\rho_o}{N}\right)^2 T^2 \sum_{\omega_1\omega_2} \int d\xi_1 \int d\xi_2 \frac{1}{i\omega_1 - \xi_1} \frac{1}{i\omega_2 - \xi_2} \qquad /22/$$

$$\frac{1}{i(\omega+\omega_2-\omega_1)\ -\lambda+g\mu_B\ M_\gamma\ H}\ \left(\bar{s}_{\alpha\gamma}\ \bar{\sigma}_{\delta_2\delta_1}\right)\left(\bar{s}_{\gamma\alpha},\ \bar{\sigma}_{\delta_1\delta_2}\right) \qquad /22/$$

The summation over the variables ω_1 and ω_2 can be performed in the usual way transforming them into integrals and the final result is

$$\Sigma^{(2)}_{\alpha\alpha},(\tilde{\omega}) = \left(\frac{J}{N}\ \rho_o\right)^2 \int d\xi_1 \int d\xi_2\ n_F(\xi_1)\left(1 - n_F(\xi_2)\right)$$

$$\frac{1}{\tilde{\omega} + \xi_2 - \xi_1 + g\mu_B\ M_\gamma\ H}\ \left(\bar{s}_{\alpha},\ \bar{\sigma}_{\delta_2\delta_1}\right)\left(\bar{s}_{\gamma\alpha},\ \bar{\sigma}_{\delta_1\delta_2}\right) \qquad /23/$$

where $\tilde{\omega} = i\omega - \lambda$ and n_F is the Fermi distribution function. Calculating the spin factors making use of the identity

$$\left(\bar{s}_{\alpha\gamma}\ \bar{\sigma}_{\delta_2\delta_1}\right)\left(\bar{s}_{\gamma',\alpha},\bar{\sigma}_{\delta_1\delta_2}\right) = 2S^z_{\alpha\gamma}\ S^z_{\gamma',\alpha'} + S^-_{\alpha\gamma}\ S^+_{\gamma',\alpha'} + S^+_{\alpha\gamma}\ S^-_{\gamma',\alpha'}, \qquad /24/$$

we obtain

$$\Sigma^{(2)}_{\alpha\alpha},(\tilde{\omega}) = \delta_{\alpha\alpha'}\left(\frac{J\rho_o}{N}\right)^2 \int d\xi_1\ n_F\ (\xi_1) \int d\xi_2 \left(1 - n_F\ (\xi_2)\right)\ .$$

$$\cdot\left\{ 2M_\alpha^2\ \frac{1}{\tilde{\omega}+\xi_2-\xi_1+g\mu_B\ M_\alpha\ H} + \left(S(S+1) - M_\alpha^2 - M_\alpha\right)\frac{1}{\omega+\xi_2-\xi_1+g\mu_B(M_\alpha+1)H}\right.$$

$$\left. + \left(S(S+1)\ - M_\alpha^2 + M_\alpha\right)\ \frac{1}{\tilde{\omega}+\xi_2-\xi_1+g\mu_B(M_\alpha-1)H}\right\} \qquad /25/$$

The integrals appearing in eq: /25/ are calculated in Appendix II. Introducing the new notation $\tilde{\omega}_{M_\alpha} = \tilde{\omega} + g\mu_B H M_\alpha$ the final result according to eqs. /25/ and /6,AII/ may be written for $\omega << kT$ as

$$\mathrm{Re}\Sigma^{(2)}_{\alpha\alpha},(\tilde{\omega}) = \left(-\alpha^{(2)}\ \tilde{\omega}_{M_\alpha} + \gamma^{(2)}\ g\mu_B\ M_\alpha H\right)\ \delta_{\alpha\alpha'}, \qquad /26/$$

where the coefficients are given by the following formulas

$$\gamma^{(2)} = \frac{1}{2}\left(2\,\frac{J}{N}\,\rho_o\right)^2 \log\frac{D}{kT} \qquad /27/$$

and

$$\alpha^{(2)} = S(S+1)\,\gamma^{(2)} \qquad /28/$$

The second order self-energy correction contains a logarithmic term, and it is multiplied by a factor, which is linear in ω and H. This correction is small in the limit $|\omega| << kT$ and $g\mu_B H << kT$, therefore the terms of higher orders in these quantities are not interesting for us.

We are going to collect the terms of this type in any order of the perturbation theory. We have learned from the calculation of the second order self-energy that the diagrams we are interested in, can be divided into two parts by cutting one pseudofermion and two electron lines /see the diagram in Fig.6./ Many of the diagrams in Fig.5. appear several times in Fig.6, but, as it will be shown, this overcounting can be eliminated.

The formal contribution of the diagram in Fig.6. denoted by $S_{\alpha\alpha'}(\tilde{\omega})$ is

$$S_{\alpha\alpha'}(\tilde{\omega}) = -\rho_o^2\,T^2 \sum_{\omega_1\omega_2} \int d\xi_1 \int d\xi_2\; \Gamma_{\delta_2\alpha\delta_1\gamma}\left(i\omega_2,\; i\omega \,|\, i\omega_1,\; i(\omega+\omega_2-\omega_1)\right)$$

$$\frac{1}{i\omega_1-\xi_1}\,\frac{1}{i\omega_2-\xi_2}\,\frac{}{i(\omega+\omega_2-\omega_1)+g\mu_B M_\gamma H}\;\Gamma_{\delta_1\gamma\delta_2\alpha'}\left(i\omega_1,\; i(\omega+\omega_2-\omega_1)\,|\,i\omega_2, i\omega\right).$$

Making use of the notation

$$\Gamma_{\delta\alpha\delta'\alpha'} = \Gamma^{(0)}\,\delta_{\delta\delta'}\,\delta_{\alpha\alpha'} + \left(\bar{S}_{\alpha\alpha'},\,\bar{\sigma}_{\delta\delta'}\right)\Gamma^{(\sigma)} \qquad /30/$$

carrying out the summations and evaluating the spin factors the following result is obtained.

$$S_{\alpha\alpha'}(\tilde{\omega}) = -\delta_{\alpha\alpha'}\rho_o^2 \int d\xi_1 \int d\xi_2\, n_F(\xi_1)\, n_F(\xi_2) \cdot$$

$$\Big\{ 2\Gamma^{(o)}\left(\xi_2,\omega|\xi_1,\omega+\xi_2-\xi_1\right)\frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1}\Gamma^{(o)}\left(\xi_1,\omega+\xi_2-\xi_1|\xi_2|\omega\right) +$$

$$+ 2M_\alpha^2\,\Gamma^{(\sigma)}\left(\xi_2,\omega\mid\xi_1,\omega+\xi_2-\xi_1\right)\frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1}\Gamma^{(\sigma)}\left(\xi_1,\omega+\xi_2-\xi_1|\xi_2,\omega\right)$$

$$+\left(S(S+1)-M_\alpha^2-M_\alpha\right)\Gamma^{(\sigma)}\left(\xi_2,\omega|\xi_1,\omega+\xi_2-\xi_1\right)\frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1+g\mu_B H}\Gamma^{(\sigma)}\left(\xi_1,\omega+\xi_2-\xi_1|\xi_2,\omega\right)$$

$$+\left(S(S+1)-M_\alpha^2+M_\alpha\right)\Gamma^{(\sigma)}\left(\xi_2,\omega|\xi_1,\omega+\xi_2-\xi_1\right)\frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1-g\mu_B H}\Gamma^{(\sigma)}\left(\xi_1,\omega+\xi_2-\xi_1|\xi_2,\omega\right)\Big\}$$

/31/

This result is similar to /25/, but now the integrals cannot be calculated so simply as in Eq. /25/, because also the vertices depend on ξ_1 and ξ_2.

All the terms proportional to kT or H have to be collected, therefore the contributions of all possible cuts have to be considered. On the other hand, it is worth mentioning that the contributions investigated here are obtained from that energy region of ξ_1 and ξ_2 where $|\xi_1|, |\xi_2| < kT$ /see Appendix II./.

Two difficulties arise in the calculation presented here:

1. Considering all of the possible cuts corresponding to the diagram in Fig. 6. some diagrams appear several times and so many diagrams are overcounted in this way. On the other hand, it can be shown, that the interesting contributions linear in H and ω cannot be ordered to definit cuts in a way one to one. Therefore the overcounting cannot be regarded as a formal procedure to collect the contributions ordered to different cuts.+

Footnote:+ A formal overcounting appeared in the works of Eliashberg [30] and Abrikosov [24], where the imaginary part of the electron self-energy has been calculated. It has been used to collect all imaginary self-energy contributions. This problem has been carefully investigated by Duke and Silverstein [31] in details up to the fourth order

2. In the expression /30/ the vertex functions occurs with such arguments that their values are not available on the basis of Sec.3.

In the limit $|\omega| << kT$ both difficulties can be avoided by applying the following tricks which are demonstrated to be true in Appendix III. considering some typical examples.

α, That cut is to be picked out, where the energy difference $\xi_2 - \xi_1$ of the electron and hole at the cut has the smallest value comparing to the similar quantities taken at all the other cuts.

β, All logarithmic terms in the vertices have to be replaced by $\log \frac{|\xi_2-\xi_1|}{D}$. /See. e.q. /11/ and /17-18/.

The contribution of the diagram in Fig. 6. has to be calculated considering the additional directions α and β.

The application of point α eliminates overcounting. On the other hand the point, β guarantees the correct values of the vertices in the logarithmic approximation.

In this way the contribution of the diagram in Fig.6. to the real part of the self-energy is

$$\mathrm{Re}\,\Sigma_{\alpha\alpha'}(\tilde{\omega}) = + \left(\frac{J\rho_o}{N}\right)^2 \int d\xi_1 \int d\xi_2\, n_F(\xi_1)\left(1 - n_F(\xi_2)\right)$$

$$\left\{ 2M_\alpha^2 \frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1} + \left(S(S+1) - M_\alpha^2 - M_\alpha\right) \frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1+g\mu_B H} \right.$$

$$\left. + \left(S(S+1) - M_\alpha^2 + M_\alpha\right) \frac{1}{\tilde{\omega}_{M_\alpha}+\xi_2-\xi_1-g\mu_B H} \right\} \frac{1}{\left(1+2\frac{J}{N}\rho_o \log \frac{D}{|\xi_2-\xi_1|}\right)^2} \qquad /32/$$

which is the modified form of eq. /51/. The terms $\log \frac{D}{|\xi_2-\xi_1|}$ would have been replaced by $\log \frac{1}{|\xi_2-\xi_1|+kT}$ in order to take into account the thermal smearing but the result of integration does not depend on this replacement. It is interesting to mention that the contribution of the spin independent part of the vertex function $\Gamma^{(o)}$ is cancelled in the logarithmic approximation.

The integrals appearing in eq. /32/ are calculated in Appendix II. /See eq. /10,AII/./ The final expression of the real part of the self-energy can be written as

$$\mathrm{Re}\,\Sigma_{\alpha\alpha'}(\omega_{M_\alpha}) = \left(-\alpha\,\tilde{\omega}_{M_\alpha} + \gamma\, g\mu_B\, M_\alpha H\right)\delta_{\alpha\alpha'} \qquad /33/$$

where the coefficients are

$$\gamma = \frac{1}{2}\,\frac{\left(2\frac{J}{N}\rho_o\right)^2 \log\frac{D}{kT}}{1 + \frac{2J\rho_o}{N}\log\frac{D}{kT}} \qquad /34/$$

and

$$\alpha = S(S+1)\gamma \qquad /35/$$

This result is the generalization of the previously obtained eqs. /26-28/ which are completed now by the characteristic factor of the Kondo problem. The latter diverges at the Kondo temperature, therefore the validity of our results is restricted to the temperature region well above the Kondo temperature.

The results in eqs. /33-35/ are adequate in the region $|\tilde{\omega}_{M_\alpha}| \ll kT$ which covers the physically most interesting part of the spectral function /see Sec.5./., where it has a maximum of width proportional to $\left(2\frac{J}{N}\rho_o\right)^2 kT$ therefore this maximum can be found in the middle of the energy region $|\omega_{M_\alpha}| \ll kT$. It is worth mentioning that the term proportional to $H \log\frac{D}{kT}$ was first pointed out by Spencer and Doniach [17] in the second order of the perturbation theory for the case $S = \frac{1}{2}$ [+] The other type of terms, proportional to $\tilde{\omega}\log\frac{D}{kT}$ has been neglected by them.

A similar logarithmic term has been found by Sólyom and one of the authors /A.Z./ [32] in the self-energy of the electrons, namely $\langle S^z\rangle \log\frac{D}{kT}$ [++] which goes to zero with magnetic field, because the magnetization $\langle S^z\rangle$ vanishes. Recently Wang and Scalapino [18] derived similar terms in the high field limit, which are proportional to $\omega \log\frac{D}{H}$ and $H \log\frac{D}{H}$.

[+] The difference by a factor 1/2 is due to a misprint in their work.

[++] It has been found that the electron self-energy is

$$\Sigma^{(2)}(\omega_n) = -\left(\frac{J}{N}\right)^2 \langle S^z\rangle\, c\,\rho_o \int \frac{d\xi}{i\omega_n + g\mu_B H - \xi}\left(\tanh\frac{\xi}{2T} - \coth\frac{g\mu_B H}{2T}\right)$$

where c is the impurity concentration. For its real part we have

$$\mathrm{Re}\,\Sigma^{(2)}(\omega + i\varepsilon) = c\left(\frac{J}{N}\right)^2 \rho_o \langle S^z\rangle \log\frac{D}{kT} + \text{non log. terms}$$

in the case of $|\omega| \ll kT$ and $\mu_B g H \ll kT$

b. Imaginary part of the self-energy

It is well known that the Korringa [33] relaxation rate is proportional to the temperature and approximately independent of the energy and magnetic field and therefore it may be expected that the imaginary part of the self-energy does not vanish at zero energy and zero magnetic field, as the real part does. This result suggests that a weak magnetic field does not affect the relaxation time, if $g\mu_B H << kT$.

The imaginary part of the self-energy occurs first in the second order of perturbation theory, i.e. in the calculation of the diagram shown in Fig. 5. In the case $H = 0$ the imaginary part of its contribution given by eq. /25/ is as follows

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega} \pm i\varepsilon) = \mp\,\delta_{\alpha\alpha'}\, 2\pi\, S(S+1) \int d\xi_1 \int d\xi_2 \left(1-n_F(\xi_1)\right)\, n_F(\xi_2)\, \delta(\tilde{\omega} + \xi_2 - \xi_1) \qquad /36/$$

The integral appearing in /36/ can be easily calculated

$$\int d\xi\; n_F(\xi)\left(1 - n_F(\tilde{\omega} + \xi)\right)\Big|_{|\tilde{\omega}| << kT} \approx kT \qquad /37/$$

so we get

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega} + i\varepsilon) = \mp\,\delta_{\alpha\alpha'}\, 2\pi\, S(S+1)\, kT \qquad /38/$$

Let us consider again the diagram in Fig.6. In the logarithmic approximation the cut exhibits those three Green's functions whose imaginary part is taken, while the real part of the vertex functions on the two sides have to be considered. The imaginary part is taken from different parts of the diagram according to the different cuts., and this eliminates the overcounting. This calculation is very similar to Abrikosov's calculation [24] of the imaginary part of the electron self-energy.

The imaginary part of the formal contribution $S_{\alpha\alpha'}(\tilde{\omega})$ of the diagram in Fig.6. can be obtained from eq. /31/

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega} \pm i\varepsilon) = \mathrm{Im}\,S_{\alpha\alpha'}(\tilde{\omega} \pm i\varepsilon) =$$

$$= \mp\,\delta_{\alpha\alpha'}\, 2\pi\,\rho_o^2 \int d\xi_1 \int d\xi_2 \left(1 - n_F(\xi_1)\right) n_F(\xi_2) \qquad /39/$$

$$\left[\Gamma^{(o)\,2}(\xi_1,0|\xi_2,\omega) + S(S+1)\;\Gamma^{(\sigma)\,2}(\xi_1,0|\xi_2,\omega)\right]\,\delta\left(\omega + \xi_2 - \xi_1\right)$$

In the case $|\tilde{\omega}| << kT$ the pseudofermion variables of the vertex functions can be neglected, therefore Abrikosov's result given in eq. /14/ can be used. Inserting eq. /14/ into eq. /39/ the following result is obtained

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\omega \pm i\varepsilon) = \mp\,\delta_{\alpha\alpha'}\,\frac{1}{2}\,\pi\,S(S+1)\left(2\,\frac{J}{N}\,\rho_o\right)^2 \cdot$$

$$\cdot\,\frac{kT}{\left(1 + 2\,\frac{J}{N}\,\rho_o\,\log\frac{D}{kT}\right)^2} \qquad /40/$$

where the integral has been calculated according to /37/.

In the opposite limit $|\tilde{\omega}| > kT$, the vertex function is not available even in logarithmic approximation. Fortunately not the vertex functions themselves, but only some integrals built up from these vertex functions are needed. It will be shown that these integrals can be obtained in the logarithmic approximation.

In this limit $|\tilde{\omega}| > kT$ eq. /39/ can be simplified to the following expression

$$\mathrm{Im}\Sigma_{\alpha\alpha'}(\tilde{\omega} \pm i\varepsilon) =$$

$$= \begin{cases} \mp\,\delta_{\alpha\alpha'}\left(2\,\frac{J}{N}\,\rho_o\right)^2 \pi \int_{-\tilde{\omega}}^{0} d\xi \left[\Gamma^{(o)2}(\xi+\tilde{\omega},0|\xi,\tilde{\omega}) + S(S+1)\;\Gamma^{(\sigma)\,2}(\xi+\tilde{\omega},0|\xi,\tilde{\omega})\right] & \text{for } \tilde{\omega} > kT \\ 0 & \text{for } \tilde{\omega} < -kT \end{cases} \qquad /41/$$

It might be learned from studying the vertex function $\Gamma(\xi + \tilde{\omega},0|\xi,\tilde{\omega})$ that this is built up by logarithmic terms of the following two types as $\log\frac{D}{|\xi+\tilde{\omega}|}$ and $\log\frac{D}{|\xi|}$.
Inserting these vertex functions into eq. /41/ integrals of the following type ought to be calculated.

$$I^{n,m}(\omega) = \int_0^{\tilde{\omega}} dx \left(\log \frac{D}{|\tilde{\omega} - x|}\right)^n \left(\log \frac{D}{|x|}\right)^m \qquad /42/$$

where n and m are integers and $x = -\xi$ Nevertheless, it will be shown that the value of this integral depends only on /n+m/ and not on n and m separately.

Really, we can write eq. /42/ as the sum of two integrals

$$I^{n,m} = \int_0^{\frac{1}{2}\tilde{\omega}} dx \left(\log \frac{D}{|\tilde{\omega}-x|}\right)^n \left(\log \frac{D}{|x|}\right)^m + \int_{\frac{1}{2}\tilde{\omega}}^{\tilde{\omega}} dx \left(\log \frac{D}{|\tilde{\omega}-x|}\right)^n \left(\log \frac{D}{|x|}\right)^m \qquad /43/$$

The second integral may be written in a similar form as the first one, if $y=\tilde{\omega} - x$ is introduced as a new variable. Let us consider now the first one. The factor containing the logarithmic term $\log \frac{D}{|\tilde{\omega}-x|}$ can be taken out of the integral up to logarithmic accoracy and the remaining integral can be calculated exactly

$$\int_0^{\frac{1}{2}\tilde{\omega}} dx \left(\log \frac{D}{|\tilde{\omega}-x|}\right)^n \left(\log \frac{D}{|x|}\right)^m = \left(\log \frac{D}{|\tilde{\omega}|}\right)^n \int_0^{\frac{1}{2}\tilde{\omega}} \left(\log \frac{D}{|x|}\right)^m dx \cong$$

$$\cong \left(\log \frac{D}{|\tilde{\omega}|}\right)^n \frac{1}{2}\tilde{\omega} \left(\log \frac{D}{\frac{1}{2}\tilde{\omega}}\right)^m \cong \frac{1}{2}\tilde{\omega} \left(\log \frac{D}{|\tilde{\omega}|}\right)^{n+m} \qquad /44/$$

where only the highest power of the logarithmic term is kept. Repeating the same procedure for the second term of eq. /43/, the following result is obtained

$$I^{n,m}(\tilde{\omega}) = \tilde{\omega}\left(\log\frac{D}{|\tilde{\omega}|}\right)^{n+m} \qquad /45/$$

which confirms our previous statement.

Let us return to the calculation of the integral in eq. /41/, As it is shown by eq. /45/ the value of the integral does not change, if the logarithmic terms $\log\frac{D}{|\tilde{\omega}-x|}$ and $\log\frac{D}{|x|}$ are replaced by $\log\frac{D}{|\tilde{\omega}|}$. Supposing that all the logarithmic terms are independent of $\tilde{\omega}$ /they are $\log\frac{D}{|x|}$ /, we can use Abrikosov's vertex function given by eq. /14/ with variable x instead of kT and we get

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega}\pm i\varepsilon) =$$

$$= \mp\,\delta_{\alpha\alpha'}\,\frac{1}{2}\,\pi\,S(S+1)\left(2\,\frac{J}{N}\,\rho_o\right)^2\int_0^{\tilde{\omega}} dx\,\frac{1}{\left(1+2\,\frac{J}{N}\,\rho_o\,\log\frac{D}{|x|}\right)^2} \quad \text{for} \quad |\tilde{\omega}| > kT \qquad /46/$$

which can be easily calculated yielding

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega}\pm i\varepsilon) =$$

$$= \mp\,\delta_{\alpha\alpha'}\,\frac{1}{2}\,\pi\,S(S+1)\left(2\,\frac{J}{N}\,\rho_o\right)^2\frac{\tilde{\omega}}{\left(1+2\,\frac{J}{N}\,\rho_o\,\log\frac{D}{\tilde{\omega}}\right)^2} \qquad /47/$$

Summarizing the results of eqs. /40/, /45/ and /47/ we have

$$\mathrm{Im}\,\Sigma_{\alpha\alpha'}(\tilde{\omega}\pm i\varepsilon) = \mp\,\delta_{\alpha\alpha'}\,\frac{1}{2}\,\pi\,S(S+1)\left(2\,\frac{J}{N}\rho_o\right)^2\begin{cases}\dfrac{\tilde{\omega}}{\left(1+2\frac{J}{N}\rho_o\,\log\frac{D}{\tilde{\omega}}\right)^2} & \text{for} \quad \tilde{\omega}>kT\\[2ex] \dfrac{kT}{\left(1+2\frac{J}{N}\rho_o\,\log\frac{D}{kT}\right)^2} & \text{for} \quad |\tilde{\omega}|<kT\\[2ex] 0 & \text{for} \quad \tilde{\omega}<-kT\end{cases} \qquad /48/$$

It is worth mentioning that we have similar forms in the limits $\tilde{\omega} > kT$ and $|\tilde{\omega}| < kT$, only the temperature has been replaced by the energy $\tilde{\omega}$.

The imaginary part of the self-energy increases as the Kondo temperature is approached from the high temperature region. This shows that the electron-impurity scattering becomes very intensive in the neighbourhood of the Kondo temperature. The inverse of the spin life-time diverges at the Kondo temperature showing that the logarithmic approximation looses its applicability in this region.

The calculation of the self-energy would be much more difficult in high magnetic field / $g\mu_B H >> kT$ / and this is beyond the scope of the present paper. It may be mentioned that in this case the magnetic field would replace the temperature in some of the logarithmic expressions e.g. $\log \frac{D}{kT}$ would be changed by $\log \frac{D}{g\mu_B H}$. Recently Wang and Scalapino [18] have calculated the inverse relaxation time up to third order and a $J^3 H \log H$ term has been found.

c. Relation between the imaginary parts of the electron and pseudofermion self-energy

The expression of the relaxation time, eq. /48/ reminds us to the relaxation time of the electrons, which according to Abrikosov's work [24] is

$$\mathrm{Im}\Sigma_{\mathrm{electron}} \left(|\tilde{\omega}| < kT\right) = \frac{N_i}{V} \frac{1}{4} S(S+1) \left(2 \frac{J}{N} \rho_o\right)^2 \pi \frac{1}{\left(1 + 2 \frac{J}{N} \rho_o \log \frac{D}{kT}\right)^2} \qquad /49/$$

where N and V stands for the number of the impurities and the volume resp.

It will be pointed out that this similarity is not an accidental one, and it might be predicted by using a classical argument counting the number of electron impurity collisions.

The scattering processes can be counted in two different ways, counting the number of the impurity pseudofermion scattering by electrons or holes w_i and the number of the electron scatterings by impurities w_e.

The first one can be given as[+]

Footnote: [+] A more accurate formula of the number of collision can be obtained making use of the results derived in Sec.6.

$$w_i = N_i (2S+1) \int \frac{e^{-\beta E}}{Z(2S+1)} \rho(E) \, |2\mathrm{Im}\, \Sigma(E)| \, dE$$

where the first term in the integral is the thermodynamic Gibbs factor and $\rho(E)$ is the spectral function given by eq. /61/. In the logarithmic approximation w_i can be approximated by /50/.

$$w_i = N_i \; |2 \; \mathrm{Im} \; \Sigma \; (\tilde{\omega} < kT) \; | \qquad /50/$$

There is no additional factor due to the population of the spin pseudofermion states for there is only one occupied pseudofermion state per impurity.

Considering the electron processes, we have to multiply the invers of the relaxation time by a factor, which decribes the population of the electron states and the probability that the final state is empty and by another factor of two due to the two possible spin orientations. The following result is obtained

$$w_e = 2V\rho_o \int_{-\infty}^{\infty} |2\mathrm{Im} \; \Sigma_{\mathrm{electron}} \; (E) \; | \; n_F(E) \; \left(1 - n_F(E)\right) \; dE \; \sim$$

$$\sim 4V\rho_o \left|\mathrm{Im} \; \Sigma_{\mathrm{electron}} \; (\omega \sim kT)\right| . \; kT \qquad /51/$$

For $w_i = {}_e$ and considering eqs. /50/ and /51/ into eq. /52/.

$$\mathrm{Im} \; \Sigma_{\mathrm{spin}} \; (\tilde{\omega} < kT) = 2\rho_o \left(\frac{N_i}{V}\right)^{-1} kT \; \mathrm{Im} \; \Sigma_{\mathrm{electron}} \; (\tilde{\omega} < kT) \qquad /52/$$

5. The pseudofermion propagator and its spectral function

In the previous section we have calculated the self-energy. The next step is the discussion of the Green's function itself. Inserting the real part of the approximated self-energy eq. /33-35/ correct in the interval $|\tilde{\omega}| \leq kT$ into the general form of the Green's function eq. /21/ we obtain the following expression

$$\mathcal{G}^{\mathrm{Lor}}_{\alpha\alpha'}(\tilde{\omega}) = \delta_{\alpha\alpha'} \, \frac{1}{\tilde{\omega}_{M_\alpha}(1 + \alpha) + 2\frac{J}{N}\rho_o \mu_B M_\alpha H - \gamma g \mu_B H M_\alpha - i\,\mathrm{Im}\,\Sigma(\tilde{\omega})} \qquad /53/$$

where the meaning of the index "Lorentzian" will be discussed later.

Introducing more physical notations this expression of the Green's function can be written in a more familiar form as

$$\mathcal{G}^{\mathrm{Lor}}_{\alpha\alpha'}(\tilde{\omega} + i\varepsilon) = \frac{z \; \delta_{\alpha\alpha'}}{\tilde{\omega} + g_{\mathrm{eff}} \; \mu_B \; M_\alpha H + \delta\omega_k \; M_\alpha + i \; \frac{1}{2\tau}} \qquad /54/$$

where the original energy variable $\tilde{\omega} = \tilde{\omega}_{M_\alpha} - g\mu_B H M_\alpha$ appears and the following notations have been introduced:

a, renormalization constant

$$z = \frac{1}{1+\alpha}\left(1 + \frac{1}{2}S(S+1)\frac{\left(2\frac{J}{N}\rho_o\right)^2 \log\frac{D}{kT}}{1 + 2\frac{J}{N}\rho_o \log\frac{D}{kT}}\right)^{-1} \cong$$

$$\cong 1 - \frac{1}{2}S(S+1)\frac{\left(2\frac{J}{N}\rho_o\right)^2 \log\frac{D}{kT}}{1 + 2\frac{J}{N}\rho_o \log\frac{D}{kT}} \cong 1 - \alpha \qquad /55/$$

where eqs. /34-35/ have been considered and on the right hand side of /55/ only the leading logarithmic terms are kept. This approximation is correct if

b, effective /renormalized/ gyromagnetic factor g_{eff}

$$g_{eff} = g(1-z\gamma) = g\left(1 - \frac{1}{2}z\frac{\left(2\frac{J}{N}\rho_o\right)^2 \log\frac{D}{kT}}{1+2\frac{J}{N}\rho_o \log\frac{D}{kT}}\right) \sim g\left(1 - \frac{1}{2}\frac{\left(2\frac{J}{N}\rho_o\right)^2}{1+2\frac{J}{N}\rho_o \log\frac{D}{kT}}\right) = (1-\gamma)g$$

/56/

where γ is given by eq. /34/.

c, renormalized Knight shift

$$\delta\omega_K = z \cdot 2\frac{J}{N}\rho_o \cdot \mu_B H = 2\frac{J}{N}\mu_B H\rho_o \qquad /57/$$

d, renormalized relaxation time τ

$$\frac{1}{2\tau} = z\,|\mathrm{Im}\,\Sigma(\omega \sim 0)| = \frac{\frac{1}{2}S(S+1)\cdot\pi\left(2\frac{J}{N}\rho_o\right)^2}{\left(1 + 2\frac{J}{N}\rho_o \log\frac{D}{kT}\right)^2} \qquad /58/$$

where the form /48/ of the imaginary part of the self-energy has been inserted.

The physical consequences of these results will be described in Sec. 7. It is interesting noticing that the renormalization of the Knight shift can be neglected up to logarithmic accuracy as it is shown by eq./57/.

The spectral representation for the Green's function is

$$\mathcal{G}_{\alpha\alpha'}(i\omega_n) = \delta_{\alpha\alpha'} \int \frac{\rho_\alpha(\tilde{\omega}')}{i\omega_n - \tilde{\omega}'} d\tilde{\omega}' \qquad /59/$$

where ρ_α is the spectral function, It can be obtained from the Green's function by analytical continuation in the energy variable as

$$\rho_\alpha(\tilde{\omega}) = \frac{1}{2\pi i} \left\{ \mathcal{G}_{\alpha\alpha}(\tilde{\omega} - i\varepsilon) - \mathcal{G}_{\alpha\alpha}(\tilde{\omega} + i\varepsilon) \right\} \qquad /60/$$

or making use of eq. /21/

$$\rho_\alpha(\tilde{\omega}) = \frac{1}{\pi} \frac{\operatorname{Im} \Sigma_\alpha(\tilde{\omega})}{\left(\tilde{\omega}_{M_\alpha} + 2\frac{J}{N}\rho_o \mu_B M_\alpha H - \operatorname{Re} \Sigma_\alpha(\tilde{\omega})\right)^2 + \left(\operatorname{Im} \Sigma_\alpha(\tilde{\omega})\right)^2} \qquad /61/$$

The spectral function satisfies the sum rule

$$\int_{-\infty}^{\infty} \rho_\alpha(\tilde{\omega})\, d\tilde{\omega} = 1 \qquad /62/$$

We have derived an approximation given by eq. /54/ for the Green's function valid in the interval $|\omega| \leq kT$. Calculating the spectral function from this approximation considering the definition /60/ a violation of the general sum rule eq. /62/ is observed, namely

$$\int_{-\infty}^{\infty} \rho_\alpha^{Lor}(\omega)\, d\omega = z \qquad /63/$$

The expressions /33-35/ and /58/ are applicable only at small values of the energy variables, therefore the validity of this spectral function is restricted to this interval. The approximated spectral function is of Lorentzian form. The violation of the sum rule eq. /63/ indicates that the spectral function has an essential part at large energies which will be called the "tail part". In this way the spectral function may be written

$$\rho_\alpha(\tilde{\omega}) = \begin{cases} \rho_\alpha^{Lor}(\tilde{\omega}) & \text{for} \quad |\tilde{\omega}| < \eta kT \\ \rho_\alpha^{tail}(\tilde{\omega}) & |\tilde{\omega}| > \eta kT \end{cases} \qquad /64/$$

where η is an arbitrary constant of the order of unity which separates the two intervals formally.

From the comparison of Eq.s /62-64/ we get a sum rule for the long tail part of the spectral function

$$\left(\int_{-\infty}^{-\eta kT} + \int_{\eta kT}^{\infty} \right) \rho_\alpha^{tail}(\tilde{\omega})\, d\tilde{\omega} = 1 - z + \left(\int_{-\infty}^{-\eta kT} + \int_{\eta kT}^{\infty} \right) \rho_\alpha^{Lor}(\tilde{\omega})\, d\tilde{\omega}$$

The aim of the next section is to prove this sum rule by making use of the calculated form of the self-energy. This turns out to be an appropriate check on the adequacy of the used approximation in Sec.4.

6. Long tail character of the spectral function and the normalization factor

The long tail part of the spectral function will be calculated on the basis of formula /61/ in the intervals $\tilde{\omega} < -\eta kT$ and $\tilde{\omega} > \eta kT$. According to eq. /48/ the imaginary part of the self-energy vanishes in the first interval, therefore the spectral function vanishes too,

$$\int_{-\infty}^{-\eta kT} \rho_\alpha^{tail}(\tilde{\omega})\, d\tilde{\omega} \simeq 0 \qquad /66/$$

The integral of the Lorentzian part of the spectral function in the appropriate interval

$$\int_{-\eta kT}^{\eta kT} \rho_\alpha^{Lor}(\tilde{\omega})\, d\tilde{\omega} = z + O\left(\frac{1}{\pi}\frac{\mathrm{Im}\,\Sigma}{\eta kT}\right) \qquad /67/$$

The correction corresponding to the integrals on the right hand side of eq. /65/ may be neglected, because Z contains terms of type $J^n \log^{n-1}$, while Im Σ contains lower order logarithmic terms i.e. according to eq. /48/ $J^n \log^{n-2}$.

At large energies, the imaginary part of the self-energy /48/ deviates from its energy independent value /for $|\tilde{\omega}| \leq kT$/ yielding the Lorentzian form of the spectral function. The asymptotic form of the spectral function for large energies is

$$\rho_\alpha^{tail}(\tilde{\omega}) = \frac{1}{\pi}\frac{\mathrm{Im}\,\Sigma(\tilde{\omega} - i\varepsilon)}{\tilde{\omega}^2} \qquad /68/$$

which is a consequence of eq. /61/, or by making use of eq. /48/ the following is obtained

$$\rho_\alpha^{tail}(\tilde{\omega}) = \frac{1}{2}S(S+1)\left(2\frac{J}{N}\rho_o\right)^2 \frac{1}{\tilde{\omega}} \frac{1}{\left(1 + 2\frac{J}{N}\rho_o \log\frac{D}{\tilde{\omega}}\right)^2} \qquad /69/$$

A schematic plot of the spectral function with long tail is given in Fig.7.

The contribution of the tail, eq. /69/ of the spectral function to the sum rule is

$$\int_{\eta kT}^{D} \rho_\alpha^{tail}(\omega)\, d\omega = \frac{1}{2}S(S+1)\left(2\frac{J}{N}\rho_o\right)^2 \int_{\eta kT}^{D} \frac{1}{\omega} \frac{1}{\left(1 + 2\frac{J}{N}\rho_o \log\frac{D}{\omega}\right)^2} d\omega =$$

$$= -\frac{1}{2}S(S+1)\left(2\frac{J}{N}\rho_o\right)^2 \left[\frac{1}{1+2\frac{J}{N}\rho_o \log\frac{D}{\omega}}\right]_{\eta kT}^{D} \cong \frac{1}{2}S(S+1)\left(2\frac{J}{N}\rho_o\right)^2 \frac{\log\frac{D}{kT}}{1+2\frac{J}{N}\rho_o \log\frac{D}{kT}} = \alpha = 1 - z$$

/70/

where the notation /55/ has been applied.

We can see easily from eqs. /66-67/ and /70/ that the validity of the sum rule /63/ is restored considering the long tail part of the spectral function. It is worth mentioning that in the logarithmic approximation this statement is independent of the special choice of the parameter η.

In Sec. 2. we have seen that the quantummechanical average /8/ of physical quantities have to be normalized by the factor

$$\langle N_s \rangle_\lambda = \frac{\mathrm{Tr}\ \rho\ N_s}{\mathrm{Tr}\ \rho} \qquad /71/$$

which is due to the population of the fictitious pseudofermion states. This normalization factor may be expressed by the spectral function as

$$\langle N_s \rangle = \sum_\alpha \int n_F\ (\tilde{\omega} + \lambda)\ \rho_\alpha\ (\tilde{\omega})\ d\tilde{\omega} \qquad /72/$$

Introducing the notation ω_R for the resonance frequency

$$\omega_R = -g_{eff}\ \mu_B H - \delta\omega_K \qquad /73/$$

the normalization factor can be written in the following form

$$\langle N_s \rangle_\lambda = Z\ e^{-\beta\lambda} \sum_\alpha p_\alpha \qquad /74/$$

where

$$p_\alpha = e^{-\beta\omega_R M_\alpha} \qquad /75/$$

The renormalization factor derived here is similar to the one obtained by Abrikosov [25], but it is now additionally multiplied by the renormalization factor Z. This modification of Abrikosov's result is due to the long tail part of the spectral function, which cannot be occupied by thermal excitations.

7. Static susceptibility

The magnetization is given by the physical average of the operator S^z. The physical average is defined by eq. /8/. Expressing S^z by the pseudofermion operators according to Eq. /4/, the appearing expectation value can be transformed to an expression of the Green function and furthermore of the spectral function. The final expression of the magnetization is the following

$$\langle S^z \rangle^{phys} = \lim_{\lambda \to \infty} \frac{1}{\langle N_s \rangle_\lambda} \sum_M M \int n_F(\tilde{\omega}) \rho_M(\tilde{\omega}) d\tilde{\omega} \qquad /76/$$

This quantitity can be calculated in a similar way as the normalization constant has been obtained. Making use of /77/ and /72-75/ the final result is

$$\langle S^z \rangle^{phys} = \frac{\sum_M M p_M}{\sum_M p_M} \qquad /77/$$

It looks like the classical result, except that the resonance frequency contains the Knight shift /57/ and the renormalized reduced gyromagnetic factor, eq. /56/. It is worth mentioning that the renormalization constants in the nominator and denominator of the physical average given by eq. /8/ cancel each other.

The static susceptibility is the derivative of the magnetization with respect to the external magnetic field. The final result may be formulated in terms of the classical expression of the susceptibility described by the Curie law, and it is denoted by $\chi^o(T,g)$ which is a function of the temperature and the unrenormalized gyromagnetic factor. The renormalized static susceptibility according to Eq. /76/ can be written as

$$\chi(T) = \chi^o\left(T, g = g_{eff}(T) + 2\frac{J}{N}\rho_o\right) \qquad /78/$$

In this formula the Knight shift and the compensation of the magnetic moment by the s-d scattering are described by a simple modification of the value of the gyromagnetic factor given by Eq. /56/. The static susceptibility obtained here can be written as a power series of the coupling constant and its first terms agree with the results previously derived by Yosida and Okiji [2] and others [3-7].

8. Conclusion

By making use of a slight modification of Abrikosov's method the static susceptibility has been calculated in the logarithmic approximation. The final result is in agreement with Hamann's result [15] well above the Kondo temperature up to the leading logarithmic terms and with the first few terms of the perturbative results derived previously.

The treatment presented here is based on the determination of the self-energy.

The real part of the self-energy in the neighbourhood of the pole of the pseudofermion Green's function contains a term proportional to the energy variable. This term has been neglected by Spencer and Doniach [17], but a similar term has been found by Scalapino and Wang in the opposite limit where the temperature can be neglected compared to the magnetic energy of the impurity spin. This term results in a renormalization constant and determines the shape of the spectral representation of the pseudofermion Green's function. The long tail character of the spectral function leads to many consequences e.g., the normalization factor in Abrikosov's method is changed, the dynamic susceptibility cannot be calculated treating only the Lorentzian part of the spectral function as it will be shown in the second part of this paper e.t.c.

The half-width of the impurity level given by Eq. /58/ is enhanced due to the Kondo effect, and that could be experimentally observed if the impurity paramagnetic resonance line can be observed separately from the electron lines. In this case the bottleneck [34] effect can be avoided in very dilute alloys, which drastically changes the experimental situation. It is worth mentioning that such an enhanced relaxation rate has not been observed yet in experiments where it should be [35]. The lack of any effect of Kondo type in these experiments has not been understood yet.

The treatment presented in this paper is restricted to the temperature region above the Kondo temperature. It is well known that from the physical point of wiev, anything essentially new does not happen at the Kondo temperature, but the applicability of our mathematical method breaks

down. In the logarithmic approximation it is supposed that the typical logarithmic term $\log \frac{T}{T_k} > 1$ /where T_K is the Kondo temperature/. Below the Kondo temperature other methods are necessary. Applying variational considerations Nam and Wing [11], Heeger et all [14], or decoupling the system of Green's function Zittartz [36] and Gurgenishvili, Nepsesian, Haradze [37] have derived expressions for the static susceptibility.

In the second part of this paper the dynamic spin susceptibility will be evaluated. The problem of the dynamical electron susceptibility and the dynamic total susceptibility are rather complicated therefore they are beyond the scope of the present papers.

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Appendix I.

We discuss very briefly, how the fictitious states which do not contain any pseudofermions, might be eliminated in formal procedures.

The trace can be written as the following sum

$$Tr = \sum_{n=o}^{2S+1} Tr^{(n)} \qquad /1/AI/$$

where $Tr^{/n/}$ corresponds to the states with number of pseudofermions, n and $Tr^{/n/}\{\rho....\}$ is proportional to $\left(e^{-\lambda/T}\right)^n$.

The physical average and the formal one can be written as

$$\langle A\rangle^{phys} = \frac{Tr^{(1)}(\rho A)}{Tr^{(1)}(\rho N_s)} = \lim_{\lambda\to\infty} \frac{\frac{Tr^{(1)}(\rho A)}{Tr^{(o)}\rho}}{\langle N_s\rangle_\lambda} \qquad /2/AI/$$

and

$$\langle A\rangle^{form} = \lim_{\lambda\to\infty} \frac{\langle A\rangle_\lambda}{\langle N_s\rangle_\lambda} = \lim_{\lambda\to\infty} \frac{1}{\langle N_s\rangle_\lambda} \frac{\sum_{n=o}^{2S+1} Tr^{(n)}(\rho A)}{\sum_{n=o}^{2S+1} Tr^{(n)}\rho} \qquad /3/AI/$$

respectively.

The formal average in the limit $\lambda \to \infty$ keeping only the terms proportional to $e^{\lambda/T}$ and 1 is the following

$$\langle A\rangle^{form} = \lim_{\lambda\to\infty} \frac{\langle A\rangle_\lambda}{\langle N_s\rangle_\lambda} = \lim_{\lambda\to\infty} \left\{ \frac{1}{\langle N_s\rangle_\lambda} \frac{Tr^{(o)}(\rho A)}{Tr^{(o)}\rho} + \right.$$

$$\left. + \frac{1}{\langle N_s\rangle_\lambda} \left[\frac{Tr^{(1)}(\rho A)}{Tr^{(o)}\rho} - \frac{Tr^{(o)}(\rho A)}{(Tr^{(o)}\rho)^2} Tr^{(1)}\rho \right] \right\} \qquad /4/AI/$$

where the first term diverges as $\lambda \to \infty$. The physical average can be expressed by the formal one comparing /3/AI/ and /4/AI/

$$\langle A\rangle^{phys} = \lim_{\lambda\to\infty} \left\{ \frac{\langle A\rangle_\lambda}{\langle N_s\rangle_\lambda} + \frac{1}{\langle N_s\rangle_\lambda} \frac{Tr^{(o)}(\rho A)}{Tr^{(o)}\rho} \left[\frac{Tr^{(1)}\rho}{Tr^{(o)}\rho} - 1 \right] \right\} \qquad /5/AI/$$

where the additional expression on the right hand side might be calculated easily, namely

a/ $Tr^{/o/}(\rho A)$ can be calculated exactly, because the interaction part of the Hamiltonian /3/ does not contribute to it.

b/ $Tr\rho = e^{-\Omega/T}$, where Ω is the sum of the contributions corresponding to the linked cluster diagrams. Ω can be written as the following sum

$$\Omega = \sum_{n=o}^{\infty} \Omega^{(n)} \qquad /6/AI/$$

where $\Omega^{(n)}$ is proportional to $\left(e^{-\lambda/T}\right)^n$ Comparing this expression, /6/AI/ with

$$Tr(\rho) = \sum_{n=0}^{\infty} Tr^{(n)}(\rho)$$

which follows from /1/AI/, we get

$$Tr^{(0)}(\rho) = e^{-\frac{\Omega^{(0)}}{T}} \quad \text{and} \quad Tr^{(1)}(\rho) = -e^{\frac{\Omega^{(0)}}{T}} \frac{\Omega^{(1)}}{T}$$

The presented procedure can be applied in all case, when there is only one impurity. In the special case, whre the identity $Tr^{(0)}(\rho A) \equiv 0$ holds due to the actual structure of the operator A, our previous result /8/ is obtained from the general formula /5/AI/.

Another method can be given for the calculation of the electron propagator, in which case $A=-iT\{\psi(x)\ \psi^+(x')\}$ The term $Tr^{(0)}(\rho A)$ appearing in /5/AI/ is proportional to the free electron propagator. Let us denote the spectral function of the electron propagator calculated in the formal way /by making use of the linked cluster theorem/, and the spectral function of the physical and free propagators resp. by $\rho_\lambda(x,x';E)$ $\rho^{phys}(x,x';E)$ and $\rho^{(0)}(x,x';E)$. According to /5/AI/ we have the following representation of the physical spectral function

$$\rho^{phys}(x,x';E) = \frac{1}{\langle N_s \rangle_\lambda} \rho_\lambda(x,x';E) + C_\lambda \rho^{(0)}(x,x';E) + O\left(e^{-\lambda/T}\right)$$

where the constant C_λ is $\langle N_s \rangle_\lambda^{-1} \left| 1 - \frac{Tr^{(1)}(\rho)}{Tr^{(0)}(\rho)} \right|$ and diverges as $e^{\lambda/T}$ in the limit $\lambda \to \infty$. /7/AI/

On the other hand, the diagonal spectral function /e.g. $x = x'$/ satisfies the sum rule

$$\int \rho^{phys}(x = x';E)\, dE = 1 \qquad /8/AI/$$

The easiest way to determine the constant is to insert eq. /7/AI/ and perform the integration.

This result can be summarized in the following manner. The scattering part of the physical propagator can be calculated by making use of Abrikosov's method, and its amplitude has to be modified by the normalization factor $\left(\langle N_s \rangle_\lambda\right)^{-1}$. The amplitude of the free part of the propagator has to be fitted according to the sum rule /8/AI/. It is vorth mentioning that in the logarithmic approximation the normalization factor, Z does not affect the scattering part of the electron propagator.+

Appendix II.

The general form of the integrals appearing in eq. /25/ is

$$I^{(o)}(w) = \int_{-D}^{D} d\xi_1 \, n_F(\xi_1) \int_{-D}^{D} d\xi_2 \left(1 - n_F(\xi_2)\right) \frac{1}{w + \xi_2 - \xi_1} \qquad /1,AII/$$

where $w = \tilde{\omega} + jg\mu_B H$ and $j=-1,0,1$. First the integral with respect to ξ_2 is transformed

$$I^{(o)}(w) = - \int_{-D}^{D} d\xi_1 \, n_F(\xi_1) \int_{-D}^{D} dn_F(y) \log \frac{|w + D - \xi_1|}{|w + y - \xi_1|} \qquad /2,AII/$$

the second one can be transformed in a similar way, and then we obtain

$$I^{(o)}(w) = - \int_{-D}^{D} dn_F(x) \int_{-D}^{D} dn_F(y) \{(x-w-D) \log |w+D-x| + (2D+w) \log |w+2D| -$$

$$- (x-w-y) \log |w+y-x| - (D+y+\omega) \log |D+y+\omega|\} \qquad /3,AII/$$

Supposing that the magnetic field is weak and the incoming energy $\tilde{\omega}$ is small enough: $|w| \ll kT \ll D$, furthermore keeping only the terms containing logarithmic expressions the integral /1,AII/ can be transformed into the following form

Footnote: +The leading logarithmic terms of the scattering amplitude are proportional to $J^{n+2}\log^n\left(\frac{D}{\omega}\right)$ and the normalization factor contains terms of type $J^{n+1}\log^n\left(\frac{D}{kT}\right)$ as it is shown in Sec.5.

$$I^{(o)}(w) = \int_{-D}^{D} dn_F(x) \int_{-D}^{D} dn_F(y)(w-x+y) \log \frac{D}{|w+y-x|} \qquad /4,AII/$$

where the term proportional to y-x is negligible because of the odd parity in the case w = o, then we get

$$I^{(o)}(w) = w \int_{-D}^{D} dn_F(x) \int_{-D}^{D} dn_F(y) \log \frac{D}{|w+y-x|} \qquad /5,AII/$$

In the logarithmic approximation the integral /5,AII/has the value $\log \frac{D}{kT}$,therefore the final result is

$$I^{(o)}(w) = w \log \frac{D}{kT} \qquad /6,AII/$$

Furthermore, calculating eq. /32/ we need the value of the following integral

$$I^{(2)}(w) = \int_{-D}^{D} d\xi_1 \, n_F(\xi_1) \int_{-D}^{D} d\xi_2 \left(1 - n_F(\xi_2)\right) \frac{1}{w+\xi_2-\xi_1} \frac{1}{1 + 2\frac{J}{N}\rho_o \log \frac{D}{|\xi_2-\xi_1|}}$$

/7,AII/

Supposing that w << kT, instead of /7,AII/ we can consider the following integral

/8,AII/

$$I^{(2)}(w) = \int_{-D}^{D} d\xi_1 \, n_F(\xi_1) \int_{-D}^{D} d\xi_2 \left(1 - n_F(\xi_2)\right) \frac{1}{w+\xi_2-\xi_1} \frac{1}{\left(1+2\frac{J}{N}\rho_o \log \frac{D}{|w+\xi_2-\xi_1|}\right)^2}$$

This integral can be calculated in a similar way as the previous one. Transforming the second and the first integrals successively we get

$$I^{(2)}(w) = -\int_{-D}^{D} d\xi_1 \, n_F(\xi_1) \int_{-D}^{D} dn_F(y) \left(2\frac{J}{N}\rho_o\right)^{-1} \left\{1 - \frac{1}{1+2\frac{J}{N}\rho_o \log \frac{D}{|w+\xi_2-\xi_1|}}\right\} =$$

$$= \frac{1}{2\,\frac{J}{N}\,\rho_o} \int_{-D}^{D} dn_F(x) \int_{-D}^{D} dn_F(y) \left\{ 1 - \frac{1}{1 + 2\,\frac{J}{N}\,\rho_o \log \frac{D}{|w+y-x|}} \right\} (w-x+y)$$

/9,AII/

where only those terms are considered, which occur in the logarithmic approximation. The final result can be written into the following form

$$I^{(2)}(w) = w \frac{\log \frac{D}{kT}}{1 + 2\,\frac{J}{N}\,\rho_o \log \frac{D}{kT}} \,. \qquad /10,AII/$$

Appendix III.

In Sec. 4. we have calculated the contribution of the diagram in Fig. 6. instead of the original self-energy diagram in Fig. 4. It has been mentioned there that the calculation of the diagram in Fig.6. is not appropriate for two reasons, but considering the directions, $\alpha - \beta$ it becomes to be correct in logarithmic approximation. The aim of the present section is to demonstrate this statement.

First, the (n+1) th order diagram in Fig.8, is considered, which contains n loops along the dotted line. The contribution of this diagram without the spin factors is

$$\left(\frac{J}{N}\,\rho_o\right)^{n+1} T^{n+1} \sum_{\omega_1} \cdots \sum_{\omega_{n+1}} \int d\xi_1 \cdots \int d\xi_{n+1} \frac{1}{i\omega_1 - \xi_1} \cdots \frac{1}{i\omega_{n+1} - \xi_{n+1}}$$

$$\cdot \frac{1}{i(\omega+\omega_1-\omega_2)-\lambda} \cdots\cdots \frac{1}{i(\omega+\omega_1-\omega_{n+1})-\lambda} \qquad /1,AIII/$$

or performing the summations we obtain

$$\left(\frac{J}{N}\,\rho_o\right)^{n+1} \int d\xi_1\, n_F(\xi_1) \prod_{j=2}^{n+1} \int d\xi_j \left(1 - n_F(\xi_j)\right) \frac{1}{i\omega + \xi_1 - \xi_j - \lambda} \qquad /2,AIII/$$

The diagram can be cut through two solid and one dotted lines n times. If we consider the diagrams in Fig.6. this diagram appears n times as there are n different possible cuts in it.

According to direction, α that cut has to be picked out, where $\xi_i - \xi_1$ has the smallest value. Dividing the integrals in /2,AIII/ into n parts in such a way that in each of them the cut /i/ is at the right place the following form is obtained

$$\left(\frac{J}{N}\rho_o\right)^{n+1} \int_{-D}^{D} d\xi_1\, n_F(\xi_1) \sum_{i=2}^{n+2} \int_{-D}^{D} d\xi_i \left(n_F(\xi_i)-1\right) \prod_{j=2}^{j=i-1} \left\{ \int_{\xi_i}^{D} d\xi_j \left(n_F(\xi_j)-1\right) \frac{1}{i\omega+\xi_1-\xi_i-\lambda} \right\} \cdot$$

$$\frac{1}{i\omega+\xi_1-\xi_j-\lambda} \prod_{k=i+1}^{k=n+1} \int_{\xi_i}^{D} d\xi_k \left(n_F(\xi_k) - 1\right) \frac{1}{i\omega+\xi_1-\xi_k-\lambda}$$

All these terms correspond to one of the general diagram in Fig.6. and furthermore the actual vertex functions on the right or left hand side may be different. This means a one to one correspondence between the terms in /3, AIII/ and the diagrams represented by Fig.6.

Supposing that $|\omega| << kT$ the energy variable ω can be neglected in integrals excepting the one with respect to ξ_i. In this way the contributions corresponding to the vertices on the left and right hand sides of the diagram in Fig.6. contain only logarithmic terms, like $\log \frac{D}{|\xi_1-\xi_i| + kT}$ as it can be seen from the following form of eq. /3,AIII/

$$\left(\frac{J}{N}\right)^{n+1} \rho_o \int d\xi_1\, n_F(\xi_1) \sum_{i=2}^{n+2} \int d\xi_i \left(n_F(\xi_i) - 1\right) \left[\rho_o \log \frac{D}{|\xi_1 - \xi_i| + kT}\right]^{i-2}$$

$$\frac{1}{\tilde{\omega} + \xi_1 - \xi_i} \left[\rho_o \log \frac{D}{|\xi_1 - \xi_i| + kT}\right]^{n-i+1} \qquad /4,AIII/$$

These logarithmic terms depend only on the difference of the energies of the electron and hole lines at the cut, as it has been stated by the direction β.

We have seen, that in this simple case of n possible cuts the method described In sec. 4. works.

Now, we calculate the diagram in Fig.9.

The contribution of this diagram can be calculated very easily and after having performed the summation the following result is obtained

$$I = \left(\frac{J}{N}\rho_o\right)^4 \int d\xi_1\, n_F(\xi_1) \int d\xi_2 \left(n_F(\xi_2) - 1\right) \int d\xi_3 \left(n_F(\xi_3) - 1\right) \int d\xi_4\, n_F(\xi_4)$$

$$\frac{1}{\tilde{\omega}+\xi_1-\xi_3} \frac{1}{\tilde{\omega}+\xi_1-\xi_2} \frac{1}{\tilde{\omega}+\xi_1+\xi_4-\xi_2-\xi_3} \qquad /5,AIII/$$

The integrals can be divided into two parts in that way that the difference of the energy variables is the smallest at the first or the second cut resp.. Then we get

$$I = I_1 + I_2 \qquad /6,AIII/$$

where

$$I_1 = \left(\frac{J}{N}\rho_o\right)^4 \int_{-D}^{D} d\xi_1\, n_F(\xi_1) \int_{-D}^{D} d\xi_2 \left(n_F(\xi_2) - 1\right) \int_{\xi_2}^{D} \left(n_F(\xi_3) - 1\right) \cdot$$

$$\cdot \int_{-D}^{D} d\xi_4\, n_F(\xi_4) \frac{1}{\tilde{\omega}+\xi_1-\xi_3} \frac{1}{\tilde{\omega}+\xi_1-\xi_2} \frac{1}{\tilde{\omega}+\xi_1+\xi_4-\xi_2-\xi_3} \qquad /7,AIII/$$

$$I_2 = \left(\frac{J}{N}\rho_o\right)^4 \int_{-D}^{D} d\xi_1\, n_F(\xi_1) \int_{-D}^{D} d\xi_3 \left(n_F(\xi_3) - 1\right) \int_{\xi_3}^{D} d\xi_2 \left(n_F(\xi_2) - 1\right) \cdot$$

$$\cdot \int_{-D}^{D} d\xi_4\, n_F(\xi_4) \frac{1}{\tilde{\omega}+\xi_1-\xi_2} \frac{1}{\tilde{\omega}+\xi_1-\xi_3} \frac{1}{\tilde{\omega}+\xi_1+\xi_4-\xi_2-\xi_3} \qquad /8,AIII/$$

Let us consider e.g. the expression /7,AIII/ This contains the following integral, which can be estimated very easily

$$\left(\frac{J}{N}\rho_o\right)^4 \int_{-D}^{D} d\xi_4 \frac{n_F(\xi_4)}{\tilde{\omega}+\xi_1+\xi_4-\xi_2-\xi_3} = \log \frac{|\xi_1-\xi_2-\xi_3+\tilde{\omega}| + kT}{|D-\xi_2-\xi_3+\xi_1+\tilde{\omega}|+kT} = \log \frac{|\xi_1-\xi_2-\xi+\tilde{\omega}|+kT}{D} \simeq$$

$$\simeq \log \frac{|\xi_1-\xi_3+\tilde{\omega}|+kT}{D} + \log\left(1 - \frac{\xi_2}{\xi_1-\xi_3+\tilde{\omega}}\right) \simeq \log \frac{|\xi_1-\xi_3+\tilde{\omega}|+kT}{D} \qquad /9,AIII/$$

where the last approximation is correct because $-1 < \frac{\xi_2}{\xi_1-\xi_3+\omega} < 0$ as $\xi_2 < \xi_3$ and so the neglected quantity is smaller than log2. Inserting /9,AIII/ into /7,AIII/and performing the integration with respect to ξ_3 the following result is obtained

$$I_1 = \left(\frac{J}{N}\rho_o\right)^4 \int_{-D}^{D} d\xi_1\, n_F(\xi_1) \int_{-D}^{D} d\xi_2 \left(n_F(\xi_2) - 1\right) \frac{1}{\omega+\xi_1-\xi_2} \int_{\xi_2}^{D} d\xi_3 \left(n_F(\xi_3) - 1\right) \cdot$$

$$\cdot \frac{1}{\omega+\xi_1-\xi_3} \log \frac{|\xi_1-\xi_3+\tilde{\omega}|+kT}{D} = \left(\frac{J}{N}\rho_o\right)^4 \int_{-D}^{D} d\xi_1\, n_F(\xi_1) \int_{-D}^{D} \left(n_F(\xi_2) - 1\right) \cdot$$

$$\cdot \frac{1}{\omega+\xi_1-\xi_2} \frac{1}{2} \log^2 \frac{|\xi_1-\xi_2| + kT}{D} \qquad /10,AIII/$$

where it has been supposed that $|\tilde{\omega}| << kT$. The integrals whithout the logarithmic factor correspond to the contribution of the lines cut by the first cut in Fig.9. As it will be shown below the factor $\frac{1}{2}\log^2 \frac{D}{|\xi_1-\xi_2|+kT}$ is due to the vertex on the left hand side in Fig.6., which vertex is represented in Fig.10. Let us calculate the contribution of this vertex in the limit $|\tilde{\omega}| << kT$, the following result is obtained

$$\int d\xi_1\, n_F(\xi_1) \int d\xi_2 \left(n_F(\xi_2) - 1\right) \frac{1}{\xi_2-i\omega-\tilde{\omega}} \frac{1}{\xi_2-\xi_1-\tilde{\omega}} =$$

$$= -\int d\xi_2 \left(n_F(\xi_2) - 1\right) \frac{1}{\xi_2-i\omega-\tilde{\omega}} \log \frac{|\xi_2-\tilde{\omega}|}{D} \sim \frac{1}{2}\log^2 \frac{|\tilde{\omega}|+kT}{D} \qquad /11,AIII/$$

Now, the direction β has to be applied and so the energy variable in the logarithmic term must be replaced by $\xi_1 - \xi_2$ and so this vertex really yields the factor required.

We have seen that the diagram in Fig.6. with bare vertex on the left hand side and with the vertex shown in Fig.10. on the right hand side gives the contribution /7,AIII/if the directions α - β are taken into account. The expression /8,AIII/ can be derived in a similar way if the second cut in Fig.9. is considered.

The treatment of these typical examples shows that the method proposed in sec. 4. for the calculation of the real part of the self-energy works well in the logarithmic approximation.

Figure Captions

Fig.1. a/ graphic representation of the vertex function
$\Gamma_{\alpha\beta\alpha'\beta'}(i\varepsilon,\ i\omega \mid i(\varepsilon+\omega_1-\omega_2),\ i\omega_2)$
b/ the contributions to the vertex function in the logarithmic approximation.

Fig.2. The graphic representations of the equations of "parquet" type for the vertex parts a Λ_1 and Λ_2. The smallest values of the energies ξ can be found at the cut /dotted-broken line/.

Fig.3. The pseudofermion self-energy diagram of the first order, which corresponds to a simple energy shift.

Fig.4. Self-energy diagram yielding the physical contribution.

Fig.5. The contribution of second order to the self-energy which is of type shown by Fig.4.

Fig.6. Diagram contributing to the self-energy in logarithmic approximation, where the cut shows the electron lines and one pseudofermion line which in the case of i, Re Σ correspond to the smallest energies ξ ii, Im Σ contributs to the imaginary part. The imaginary parts of the vertexes are neglected.

Fig.7. The schematic plot of the pseudofermion spectral function showing a maximum of Lorentzian form and an additional long tail at large positive energy values.

Fig.8. Self-energy diagram of order /n+1/ with n possible cuts denoted by dotted broken lines.

Fig.9. Diagram of fourth order with two possible cuts.

Fig.10. Vertex correction of second order appearing as the vertex on right hand side in the general representation /given by Fig.6./ of the diagram in Fig.9. considering the cut 1.

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FIG. 1/a.

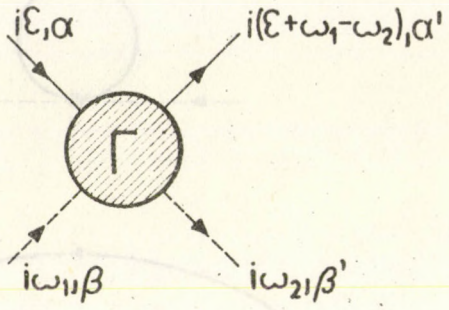


FIG. 1/b.

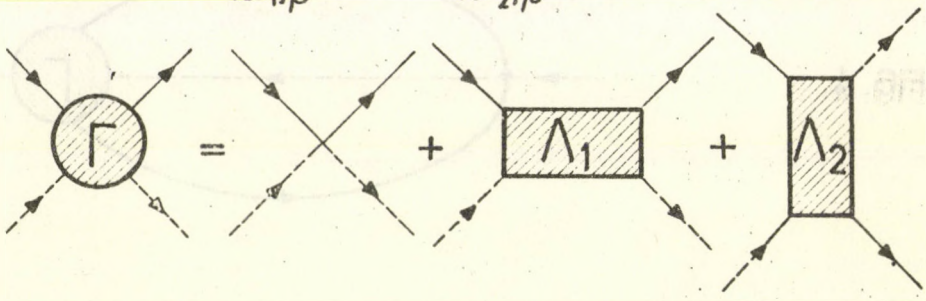


FIG. 2/a.

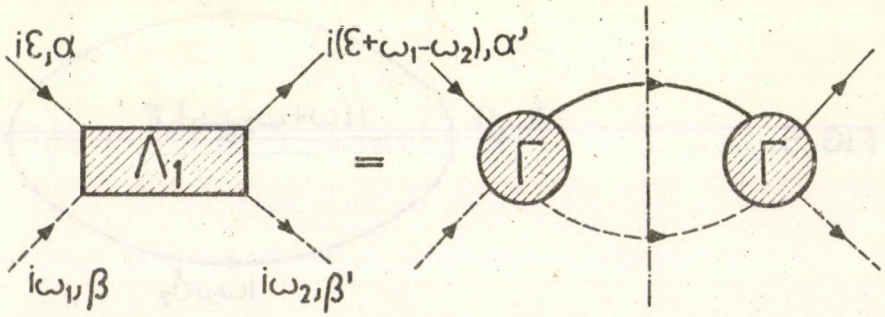


FIG. 2/b.

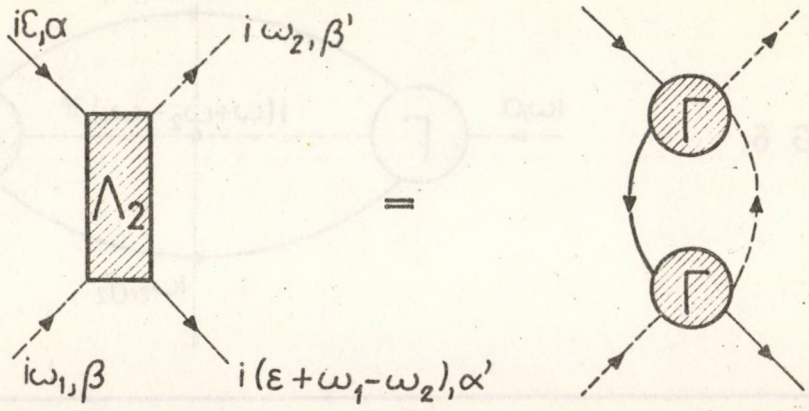
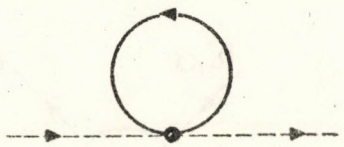


FIG. 3.



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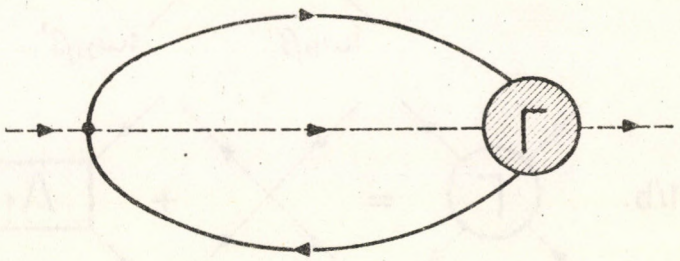


FIG. 5.

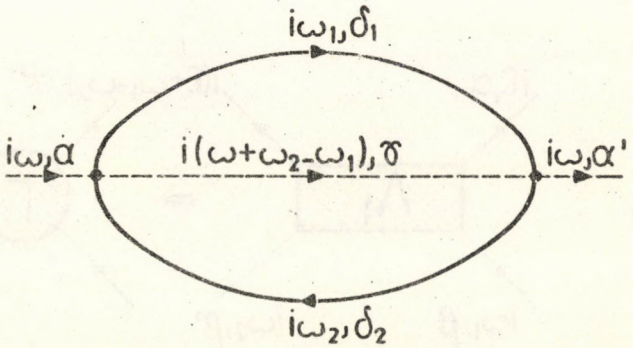


FIG. 6.

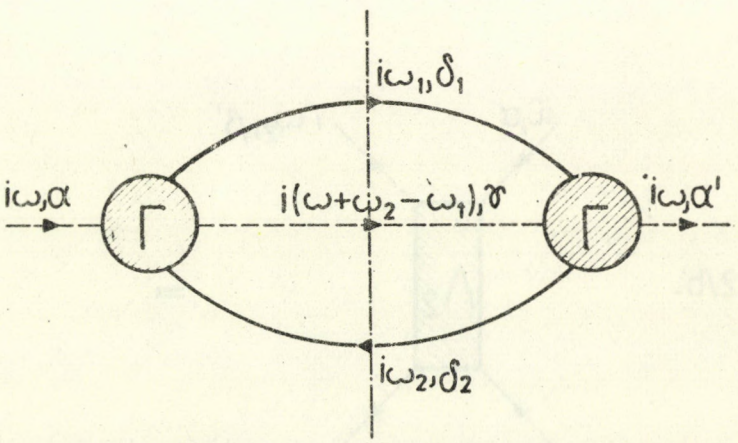


FIG. 7.

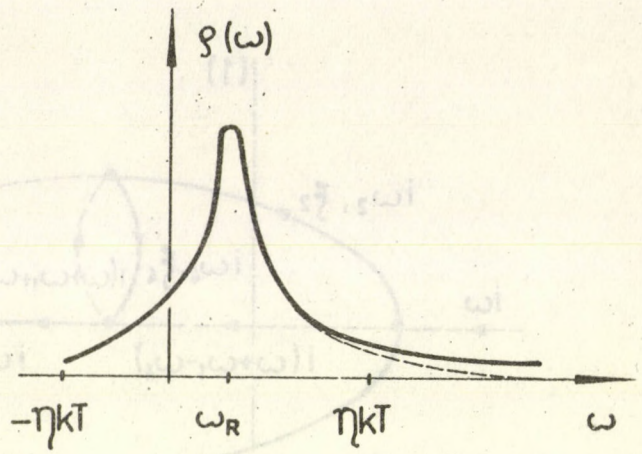
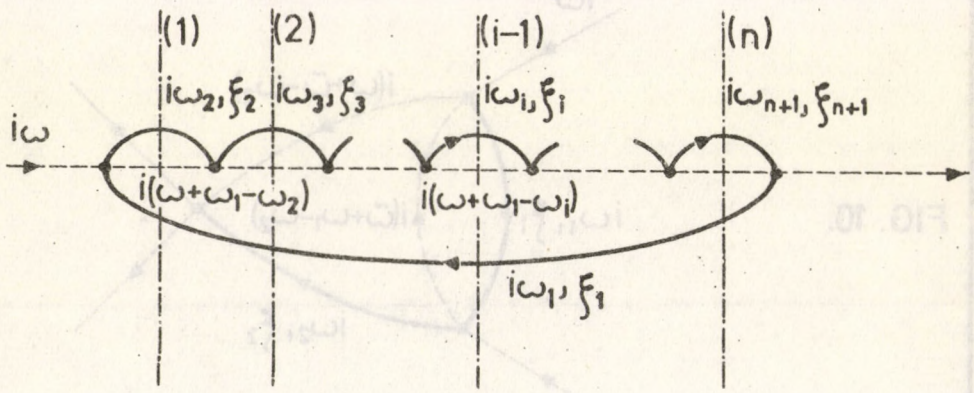

ρ(ω)
-ηkT
ω_R
ηkT
ω

FIG. 8.


(1)
(2)
(i-1)
(n)
iω
iω2, ξ2
iω3, ξ3
iωi, ξi
iωn+1, ξn+1
i(ω+ω1-ω2)
i(ω+ω1-ωi)
iω1, ξ1

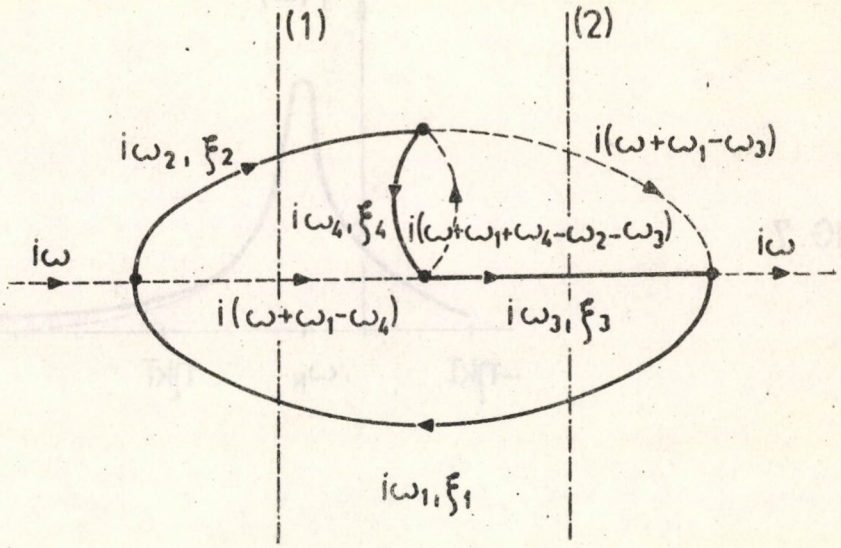

(1)
(2)
iω2, ξ2
i(ω+ω1-ω3)
iω4, ξ4
i(ω+ω1+ω4-ω2-ω3)
iω
iω
i(ω+ω1-ω4)
iω3, ξ3
iω1, ξ1

FIG. 9.

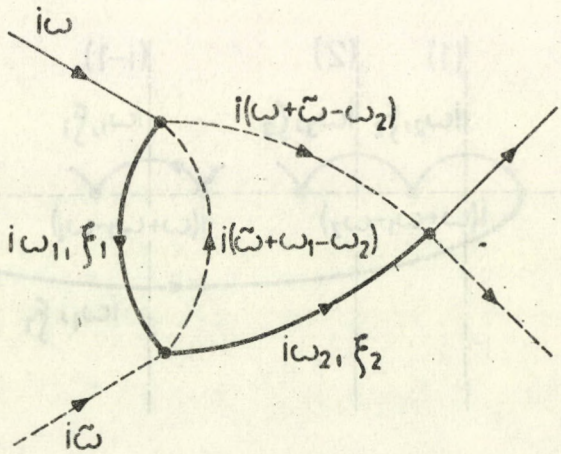

iω
i(ω+ω̃-ω2)
iω1, ξ1
i(ω̃+ω1-ω2)
iω2, ξ2
iω̃

FIG. 10.

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